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Structural, spin, and orbital phase transitions in LaOFeAs: I. Total energy calculations WEI KU, CHI-CHENG LEE, WEI-GUO YIN, Brookhaven National Laboratory — Recent experimental studies on iron pnictides showed the existence of local Fe magnetic moments even in the superconducting phase, indicating strong fluctuations in a short time scale. We report a investigation of the local electron-lattice and electron-spin couplings via total energy calculations within first-principles density functional theory. Strong coupling in both channels were found to be closely tied to a ferro-orbital order, which drives the structure transition and the stripy magnetic (SDW) transition at high temperature in the undoped system. We suggest that this orbital degree of freedom leads to stronger coupling upon doping and thus possible enhancement of superconductivity.

Prefer Oral Session
 Prefer Poster Session

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